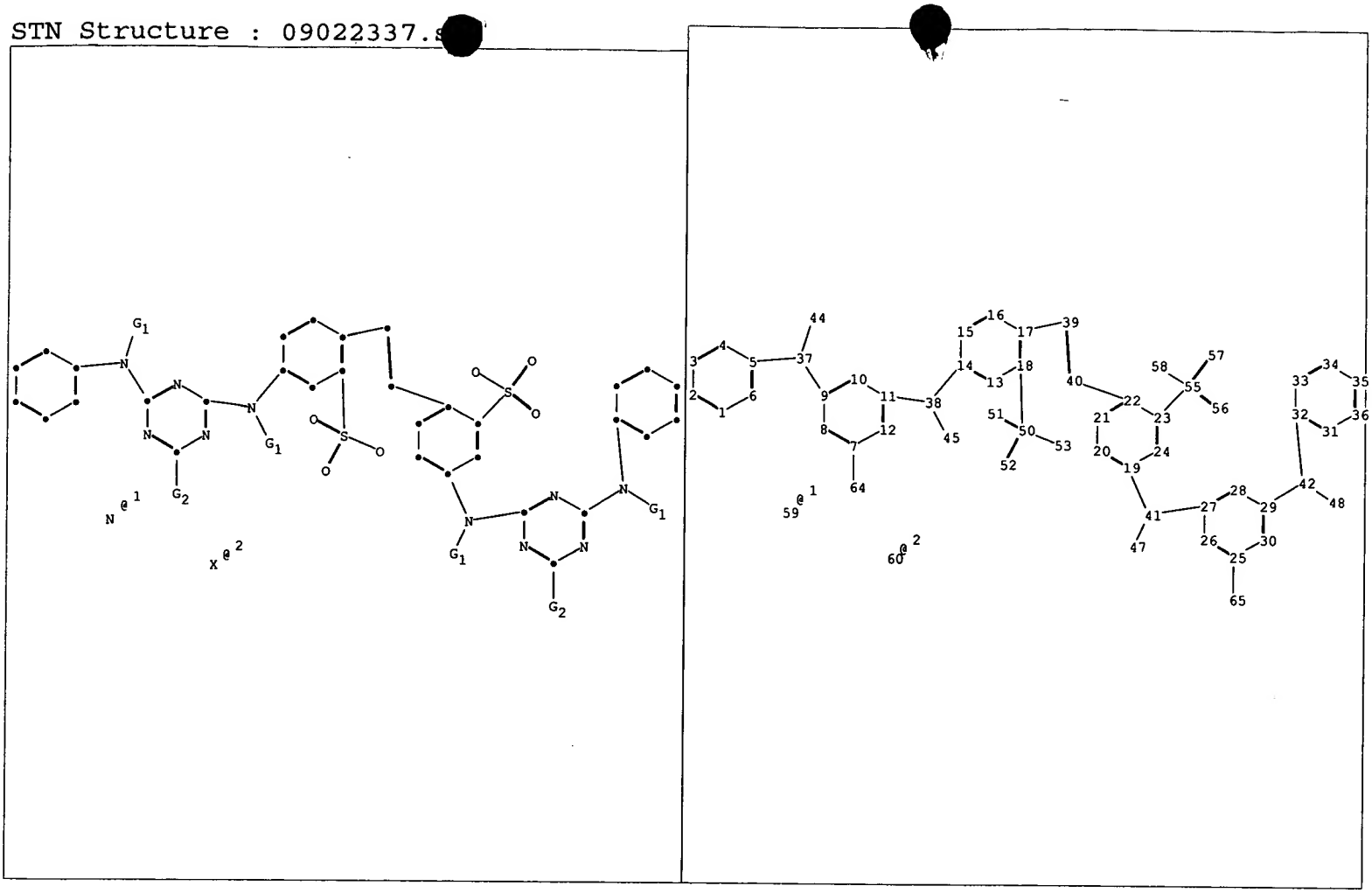
STN Structure : 09022337.s



chain nodes :
37 38 39 40 41 42 44 45 47 48 50 51 52 53 55 56 57 58
60 64 65
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21
22 23 24 25 26 27 28 29 30 31 32 33 34 35 36
ring/chain nodes :
59
chain bonds :
5-37 7-64 9-37 11-38 14-38 17-39 18-50 19-41 22-40 23-55 25-65
27-41 29-42 32-42 37-44 38-45 39-40 41-47 42-48 50-51 50-52
50-53 55-56 55-57 55-58
ring bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14
13-18 14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23
23-24 25-26 25-30 26-27 27-28 28-29 29-30 31-32 31-36 32-33
33-34 34-35 35-36
exact/norm bonds :
5-37 7-64 9-37 11-38 14-38 18-50 19-41 23-55 25-65 27-41 29-42
32-42 37-44 38-45 41-47 42-48 50-51 50-52 50-53 55-56 55-57
55-58
exact bonds :
17-39 22-40 39-40
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12 13-14
13-18 14-15 15-16 16-17 17-18 19-20 19-24 20-21 21-22 22-23
23-24 25-26 25-30 26-27 27-28 28-29 29-30 31-32 31-36 32-33
33-34 34-35 35-36
isolated ring systems :

containing 1 : 13 : 1[redacted] 25 : 31 :

G1:H,CH3

G2:[*1],[*2]

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom
10:Atom 11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom
18:Atom 19:Atom 20:Atom 21:Atom 22:Atom 23:Atom 24:Atom 25:Atom
26:Atom 27:Atom 28:Atom 29:Atom 30:Atom 31:Atom 32:Atom 33:Atom
34:Atom 35:Atom 36:Atom 37:CLASS 38:CLASS 39:CLASS 40:CLASS
41:CLASS 42:CLASS 44:CLASS 45:CLASS 47:CLASS 48:CLASS 50:CLASS
51:CLASS 52:CLASS 53:CLASS 55:CLASS 56:CLASS 57:CLASS 58:CLASS
59:CLASS 60:CLASS 64:CLASS 65:CLASS